Bending stiffness calculation for nanosize structures

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ABSTRACT Advances in high technologies using nanometer-size structures, such as carbon nanotubes, require calculation of mechanical properties for the objects of the nanosize scale level. Majority of the theoretical mechanical models for nanoobjects is based on the macroscopic equations of theory of elasticity. This gives the questions about applicability of the quantities obtained from the macroscopic experiments to the nanoscale objects or about necessity of corrections taking into account the scale effects. The presented paper is devoted to theoretical investigation of the influence of the scale effects on the bending stiffness of a nanocrystal, which is extended in one direction and has a limited number of atomic layers in another direction. Ambiguity of the bending stiffness due to the ambiguity of the size definition for the nanosize object is discussed. It is shown that appropriate definition of the crystal thickness allows using conventional formula for the bending stiffness, which is known from continuum theory of elasticity.

Keywords bending stiffness; mechanical properties; nanostructures.

NOMENCLATURE

a_{jn} = distance between the neighboring atoms in each layer
b_{jn} = distance between the neighboring atoms in different layer
C = stiffness of the interatomic bond
D = bending stiffness
E = Young's modulus
$F(r)$ = force of interaction between two atoms, separated by the distance r
H = nanocrystal thickness
h_{jn} = interlayer distance
$\mathcal{J}$ = number of layers in the x direction
j = number of the vertical layer
M = bending moment
N = number of layers in the y direction
n = number of the horizontal layer
Q_n = force, applied to atoms located at crystal end-walls
α = angle between the neighboring layers
β = curvature

INTRODUCTION

Recent advances in nanotechnologies require development of adequate analytical models for analysis of mechanical deformation for the objects of nanometer scale level. The majority of existing theoretical models are based on equations of continuum theory of elasticity. The values of the elastic moduli are usually taken from macroscopic experiments. However, a lot of researchers have noted inconsistency between the values of the elastic moduli obtained from micro- and macro-experiments (see, for example, Bykov and Konovalov[1] and Bajdarovtsev *et al.*[2]). In Krivtsov and Morozov,[3] influence of the number of atomic layers on the Young modulus and Poisson's ratio of a perfect single-crystal is investigated. It is shown that reduction in the number of the layers leads to decreasing the Poisson's ratio and increasing the Young modulus of the crystal. For the most thin films,

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containing only two atomic layers, these moduli can differ by two times from their macroscopic values. The results of the paper [3] confirm the necessity of taking into account the scale effects while applying the methods of continuum mechanics to nanosize objects. The aim of the presented paper is to investigate theoretically the scale effect for bending stiffness of thin nanocrystalline structures. The interest to these problems is connected with the necessity of investigation of the mechanical deformation of nanotube devices, which are used intensively in the recent years in nanotechnology developments.[4–7] Engineering materials and structures at the nanoscale are expected to play a key role in the production of the next generation of electronic devices such as single electron transistors, terabit memories, quantum computers, and etc.

DESCRIPTION OF THE MODEL

Let us consider a two-dimensional single crystal shown in Fig. 1. For the sake of simplicity we use hexagonal close-packed lattice. In the undistorted state, the lattice consists of equilateral triangles with an edge $a = b = a_0$. It is known that the considered crystal lattice is the only stable two-dimensional lattice for the most types of pair interactions. The crystal possesses $N \geq 2$ atomic layers in the y direction and $\mathcal{J} \gg N$ layers in the x direction. Each atom interacts only with its nearest neighbors, as it is shown in the figure. Forces Q_n are applied to atoms located at crystal end-walls, where n is the number of the horizontal layer, containing the specified atom ($n = 1, 2, \ldots, N$). These forces are changing linearly with y coordinate, keeping the zero average value of the overall force acting on the end-wall, so that we can consider

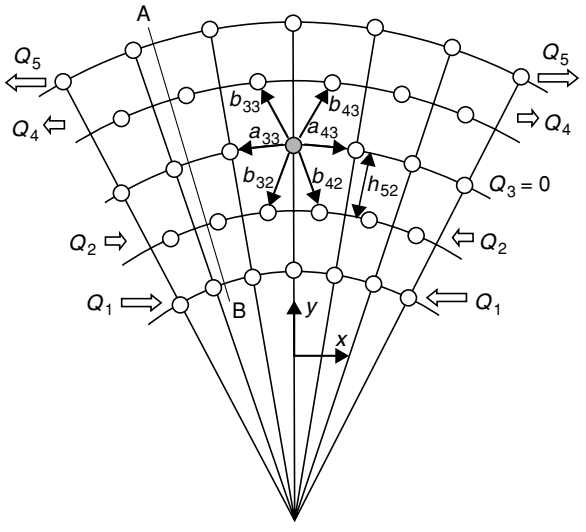

Fig. 1 Bending of the nanocrystalline strip.

the macroscopic boundary conditions as an action of a pure moment (without tensile stress):

$$\sum_{n=1}^{N} Q_n = 0, \quad \sum_{n=1}^{N} R_n Q_n = M \tag{1}$$

where R_n is the distance between the 1st and nth horizontal atomic layers in the undistorted state of the crystal. The geometrical state of the deformed crystal can be determined uniquely by the distance a_{jn} between the neighboring atoms in each layer and by the distance b_{jn} between the neighboring atoms in the different layers. Indexes j, n denote numbers of atomic layers in the directions x and y, respectively (Fig. 1). It is easy to see that the interlayer distance h_{jn} can be obtained from the geometrical relation $h_{jn}^2 = b_{jn}^2 - a_{jn}^2/4$ and in the undistorted state $h_0 = (\sqrt{3}/2)a_0$. It can be shown that $R_n = (n-1)h_0$ and the forces Q_n, which satisfy conditions Eq. (1) can be represented in the form

$$Q_n = \frac{4\sqrt{3}M(2n - N - 1)}{a_0(N-1)N(N+1)} \tag{2}$$

Let $F(r)$ be the force of interaction between two atoms separated by the distance r. Supposing the deformations to be small (in the figure the displacements are enlarged for better visibility), let us use the linear approximation for the forces of the atomic interaction

$$F(a_{jn}) = C\Delta a_{jn}, \quad F(b_{jn}) = C\Delta b_{jn}, \quad C \stackrel{\text{def}}{=} F'(a_0) > 0 \tag{3}$$

where C is the stiffness of the interatomic bond, $\Delta a_{jn} \stackrel{\text{def}}{=} a_{jn} - a_0$, $\Delta b_{jn} \stackrel{\text{def}}{=} b_{jn} - a_0$. This linearization is valid here because in the continuum mechanics the elastic moduli usually are determined from the linear theory as well. Let us note, that the suggested approach can be realized without assumption about the linearity of the elastic bonds; the relevant complications are of the technical nature only. Equations of equilibrium for the crystal lattice give the following system of recurrent equations for quantities Δa_{jn}, Δb_{jn}, and Q_n

$$\begin{aligned}
&\Delta a_{j,n} + \frac{1}{2}(\Delta b_{j,n} + \Delta b_{j,n-1}) = \Delta a_{j-1,n} + \frac{1}{2}(\Delta b_{j-1,n} + \Delta b_{j-1,n-1})] \\
&\Delta b_{j,n} + \Delta b_{j-1,n} = \Delta b_{j,n-1} + \Delta b_{j-1,n-1} \\
&\Delta a_{l,n} + \frac{1}{2}(\Delta b_{l,n} - \Delta b_{l-1,n} + \Delta b_{l,n-1} - \Delta b_{l-1,n-1}) = \frac{Q_n}{C}, \quad l = 1, 2 \\
&\Delta a_{\mathcal{J}-l,l} + \frac{1}{2}(\Delta b_{\mathcal{J}-l,n} - \Delta b_{\mathcal{J}-l+1,n} + \Delta b_{\mathcal{J}-l,n-1} - \Delta b_{\mathcal{J}-l+1,n-1}) = \frac{Q_n}{C}
\end{aligned} \tag{4}$$

By solving these equations one can obtain

$$\Delta b_{jn} = 0, \quad \Delta a_{jn} = \frac{Q_n}{C} \tag{5}$$

BENDING STIFFNESS DETERMINATION

We now mentally cut the crystal by a vertical straight line AB (Fig. 1). According to Eqs (2) and (5), the total normal force acting from one part of the crystal onto another part is equal to zero; the resultant bending moment can be calculated by formula (1) and is equal to M. As it can be seen from formulae (2) and (5) the increments of the interatomic distances Δa_{jn} are linear functions of the layer number n in the direction y and do not depend on the layer number j in the direction x. This means that the atomic layers in the direction y remain straight during the deformation and angles between the neighboring layers are equal. Then the angle between the neighboring layers α and the corresponding curvature β can be determined as following

$$\alpha \stackrel{\text{def}}{=} \frac{\Delta a_{jn}/2 - \Delta a_{j1}/2}{h_0(N-1)}, \quad \beta \stackrel{\text{def}}{=} \frac{\alpha}{a_0/2} \tag{6}$$

The bending stiffness of the monocrystal, according to Eqs. (2), (5) and (6) has the form

$$D \stackrel{\text{def}}{=} \frac{M}{\beta} = \frac{Ca_0^3}{16}(N-1)N(N+1) \tag{7}$$

An attempt to express the bending stiffness in the terms of macroscopic parameters meets with difficulties connected with the ambiguity for determination of the nanocrystal thickness H.[3] On the one hand, the nanocrystal thickness can be defined as the distance between the atomic layers at the opposite end-walls: $H=(N-1)h_0$; on the other hand, it is quite reasonable to determine the crystal thickness as a product of the number of layers by the thickness of a single layer, which results in the formula $H=Nh_0$. Since it is difficult to choose between the definitions suggested above, let us use the following definition for the nanocrystal thickness[3]

$$H \stackrel{\text{def}}{=} N_* h_0, \quad N-1 \le N_* \le N \tag{8}$$

where N_* is the dimensionless parameter reflecting an arbitrariness in the determination of H. As it shown in Ref. [3], Young's modulus E_1 corresponding to the tension along the direction in which the monocrystalline strip is long can be obtained by the formula

$$E_1 = \frac{N}{N_*}E_\infty, \quad E_\infty = \frac{2C}{\sqrt{3}} \tag{9}$$

where E_∞ is the value of the Young modulus for the infinite crystal.[8,9] In the current paper the strip has final size in x direction, but it is postulated that the number of the atomic layers in this direction is big enough to use formulae (9). Formulae (8), (9) allow to express the bending stiffness (7) of the nanocrystalline strip in the terms of the macroscopic parameters

$$D = \frac{E_1 H^3 (N^2-1)}{12N_*^2} \tag{10}$$

DISCUSSION AND CONCLUDING REMARKS

It is known from the experimental data that the bending stiffness for the single-walled nanotubes is 25 times smaller then it is predicted by the continuum theory of elasticity.[10] Indeed, from the classical atomic consideration it follows that single atomic layer should have no bending stiffness at all. That is why in the bending problems the reasonable formula for N_* should produce zero bending stiffness for the case $N=1$ (the tiny bending stiffness recorded in the experiments is connected with effects that are not taken into account by the presented model). Let us consider two representations of N_*, which satisfy the mentioned condition.

Let us consider first that $N_*=N$. Then $E_1=E_\infty$ and the bending stiffness is given by the formula

$$D = D_\infty\left(1-\frac{1}{N^2}\right), \quad D_\infty = \frac{E_\infty H^3}{12}, \quad H = Nh_0 \tag{11}$$

Here D_∞ is the value for the bending stiffness from the macroscopic theory of elasticity. According to formula (11) the bending stiffness of the nanocrystal is varying in the limits of $0 \le D \le D_\infty$. Variation of the bending stiffness with the number of the layers is illustrated by Fig. 2, where dependence of parameter $k=D/D_\infty$ on N is shown. For the small values of N the stiffness depends essentially on the number of the layers. For the greater values of N the stiffness becomes greater tending for $N\to\infty$ to the value known from the macroscopic theory of elasticity. On the other hand, let us assume that $N_* = N\sqrt[3]{1-(1/N^2)}$. Note that this definition satisfies the inequality (8): $N-1 \le N_* \le N$. The formula for the bending stiffness in this case takes the form

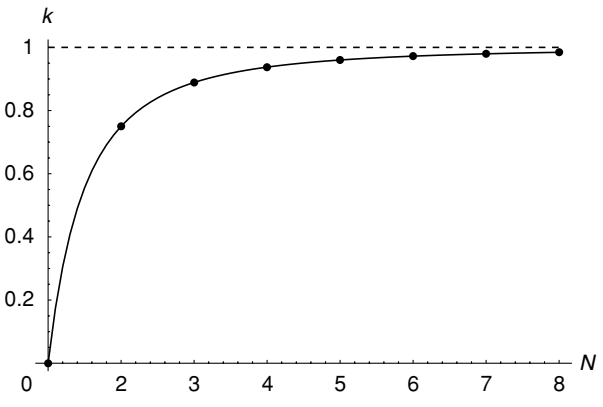

Fig. 2 Variation of the bending stiffness with the number of layers.

$$D = \frac{E_\infty H^3}{12} \equiv D_\infty, \quad H = Nh_0\sqrt[3]{1 - \frac{1}{N^2}} \tag{12}$$

Thus formula (12) for the bending stiffness exactly coincides with the one known from the theory of elasticity. Formula (12) for the strip thickness for the greater values of N coincides with the value Nh_0, corresponding to the previous case. For the small N formula (12) gives the thickness values smaller then Nh_0, and finally it vanishes for $N=1$, which is consistent with the thesis that a single-layer crystal has no bending stiffness at all.

An alternative way of the bending stiffness determination is the solution of the problem of the nanocrystalline strip deformation when it is bent into circle (representing cross-section of the nanotube). The strip should be long enough to consider the deformations as small. This problem has little bit more complicated geometry, but advantage of such statement is that it does not need any assumptions about the external load distribution. The formulae for the bending stiffness, which can be obtained from the solution of this problem, are equal to formulae (10–12).

In paper [4] the problem of bending stiffness determination for nanotubes was considered in a quasi-continuum statement. In the paper the bending stiffness was determined for several selected values of N. The same values for stiffness can be obtained from the general formula (11). The strip thickness in [4] was taken as $H=h_0N$, which results in a discrepancy with the stiffness formula known from the theory of elasticity. However, as it was shown before, alternative definition for the strip thickness allows the use of the macroscopic formula for the bending stiffness without any modifications.

The results listed in this paper are obtained on the basis of a rather simplified model. However, they can be easily generalized for other, more exact laws of interaction. In the present study we took into account only the interaction of neighboring atoms in the crystal lattice. It can be shown that allowance for further neighbors' leads to the enhanced effect of the scale factor, especially in the three-dimensional case. Thus, the concepts of classical continuum mechanics, including those of the elasticity theory, must be used with great care in the case of their application to nanoobjects. It is necessary to take into account the variation of mechanical characteristics when scales of objects under consideration approach nanometers.

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